

Density matrix renormalization group approach of the spin-boson model

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We propose a density matrix renormalization group approach to tackle a two-state system coupled to a bosonic bath with continuous spectrum. In this approach, the optimized phonon scheme is applied to several hundred phonon modes which are divided linearly among the spectra. Although DMRG cannot resolve very small energy scales, the delocalized-localized transition points of the two-state system are extracted by the extrapolation of the flow diagram results. The phase diagram is compared with the numerical renormalization group results and shows good agreement in both Ohmic and sub-Ohmic cases.

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I. INTRODUCTION

The density matrix renormalization group (DMRG) is an important tool for studying the strongly correlated systems in low dimensions.^{1,2} In the past decade, one significant limitation of DMRG—finite basis requirement in the model which involves infinite degree of freedom, e.g., phonon states, was circumvented by a controlled truncation technique.³ This technique is applied to many models, typically, such as 1D Holstein model,³ 1D Holstein-Hubbard model,⁴ spin Peierls model,⁵ and spin-boson model.⁶ The main idea of this technique, controlled truncation, is realized by the density matrix approach which is useful for finding the most probable states of the truncated system. By its light, the infinite Hilbert space can be reduced to governable dimensions without significant loss of accuracy. However, the truncation technique is originally designed for the systems involving just one phonon mode, i.e., the Einstein model. The direct application of this technique to the spin-boson model with a continuous spectrum of phonon modes, is not very successful.⁶ For instance, in the case of Ref. 6, the number of phonon modes were limited to $N = 18$, the physics of this highly discrete model may be unreliable. Furthermore, the number of states of each phonon mode kept is $m = 2$, the truncation error is relatively large and no convincing result on the delocalized-localized transition was found.⁶ These limitation implies that, to handle the system with many phonon modes in a DMRG treatment, one needs to develop an improved truncation technique. This is the motivation of the present paper.

Here, let us briefly introduce the spin-boson model. The spin-boson model is an important toy model in the study of dissipative quantum systems. Its Hamiltonian is given by (set $\hbar = 1$)^{7,8}

$$H = \frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \sum_i \omega_i a_i^\dagger a_i + \sigma_z \sum_i \lambda_i (a_i + a_i^\dagger), \quad (1)$$

where the Pauli matrices $\sigma_{x,z}$ describe a two-state system, a_i^\dagger and a_i are phonon creation and annihilation operators with frequencies ω_i for the i -th phonon modes, ϵ is an additional bias (asymmetry), Δ is the bare tunneling splitting, and λ_i represents the coupling between the

two-state system and the i -th phonon mode. Generally, the so-called bath spectral function

$$J(\omega) = \pi \sum_i \lambda_i^2 \delta(\omega - \omega_i) \quad (2)$$

completely determine the solutions of the spin-boson model. With an energy cutoff ω_c , i.e., discards the high energy modes, the bath spectral function has a power-law form

$$J(\omega) = \frac{\pi}{2} \alpha \omega^s \omega_c^{1-s}, \quad (3)$$

where α is a dimensionless coupling constant which characterizes the dissipation strength, $0 < s < 1$, $s = 1$, and $s > 1$ represent sub-Ohmic, Ohmic, and super-Ohmic dissipation, respectively. The primary purpose of the spin-boson model is to study the effect of the environment on quantum tunneling of the two-state system. Here the environment is modelled as a collection of harmonic oscillators, which serves as the origin of dissipation.^{7,8} Intuitively, the presence of the environment will make the tunneling particle as a “dressed” one, just like the electron in a polaron-phonon (or exciton-phonon) system, and therefore its quantum tunneling decreases as the coupling increases. One important issue in spin-boson model is to study the phonon-induced localization (also stated as delocalized-localized transition), i.e., how quantum tunneling dies out as the coupling (or the dissipation) increases.^{7,8,9,10,11,12,13,14,15,16} Such a delocalized-localized transition at $T = 0$ is now considered as some kind of quantum phase transition called boundary phase transition.^{17,18}

In general, the Hamiltonian of the spin-boson model cannot be solved exactly, especially in the sub-Ohmic case.⁸ The delocalized-localized transition has been widely studied by various methods with different approximations, yet a consensus on the delocalized-localized transition in sub-Ohmic case is still lacking. By integrating out the bath degrees of freedom, the spin-boson model was mapped to an Ising model and the localized transition was predicted to exist for $s \leq 1$ (i.e., in both Ohmic and sub-Ohmic cases).^{9,10} However, the path-integration with the so-called noninteracting blip approximation (NIAP) and the adiabatic renormalization

predicted that no delocalized-localized transition happens in the sub-Ohmic case.⁷ On the other hand, in the sub-Ohmic case, variational calculations, flow equation method, and other perturbation calculations predicted a discontinuous delocalized-localized transition,^{10,12,13,14} while the non-perturbative numerical renormalization group (NRG) calculation shows a continuous one.¹⁵ Recently, the authors showed that the discontinuous transition in the sub-Ohmic case obtained by the variational calculation is simply an artifact of the variational scheme due to the fact that the energy of the variational ground state can no longer be lower than the energy of the trial ground state (displaced-oscillator state).¹⁹ While this result sheds some lights on the problem, the discrepancy between various treatments mentioned above has not yet been resolved. In addition, although the NRG approach is regarded as the most powerful tool for treating the phase transition, the error due to discretization in numeric calculation has to be considered.¹⁴ Under this sense, the delocalized-localized transition is necessary to study by another non-perturbative method, i.e., DMRG. We hope that this paper will be helpful for resolving the discrepancy.

The organization of this paper is as follows. In the following section, we propose a finite system DMRG approach with controlled truncation technique to the spin-boson model, a thousand phonon modes can be treated. In Sec. III, we determine the DMRG parameters and discuss the very small energy scales limitation of our treatment. Sec. IV suggests a extrapolation scheme to circumvent the very small energy scales limitation. The delocalized-localized transition points of the spin-boson model, which is associated to the very small energy phonon modes, are obtained by extrapolation of “pseudo-critical” points. Conclusion is given in the last section.

II. THE FINITE SYSTEM DMRG ALGORITHM OF THE SPIN-BOSON MODEL

Here we present a finite system DMRG algorithm with the optimized truncation of multi-modes phonon space to treat the spin-boson model whose bosonic bath involves several hundred phonon modes. The key strategy of the algorithm is that one represents a single phonon mode as a site. The spin-boson model therefore becomes a finite-size chain. In this case, finite system DMRG is naturally applied to this model since it is appropriate to reduce the environment error with sweeping processes.²⁰ To reach this, we must divide the frequency spectrum into N intervals, i.e., $[\nu_{i-1}, \nu_i]$, where $i = 1, \dots, N$, $\nu_i - \nu_{i-1} = \nu_{i+1} - \nu_i$, $\nu_0 = 0$, $\nu_N = \omega_c = 1$, and $\omega_i = (\nu_i + \nu_{i-1})/2$. In other words, the frequency spectrum is divided linearly. The corresponding coupling parameters λ_i can be obtained by the spectral function

(2) and (3)

$$\lambda_i^2 = \frac{1}{\pi} \int_{\nu_{i-1}}^{\nu_i} J(\omega) d\omega = \frac{\alpha \omega_c^{1-s}}{2(s+1)} (\nu_i^{s+1} - \nu_{i-1}^{s+1}). \quad (4)$$

Suppose that N_b bare phonon states ($|0\rangle, |1\rangle, \dots, |N_b-1\rangle$) are sufficient to represent one phonon mode accurately, therefore we can limit N_b bare phonon states in each phonon site. Using the controlled reduction technique,³ the dimension of each phonon mode can be further reduced to m where $m < N_b$. However, even though $m = 2$ is quite large for a dozen phonon modes, as in the treatment by Nishiyama.⁶ In this case, the number of phonon modes that can be treated is seriously restricted. Our solution to this problem is to truncate a set of phonon sites with the density matrix approach within each DMRG step, i.e., we do not optimized phonon modes individually. The truncated multi-phonon sites can be continuously optimized by the sweeping of the finite system DMRG algorithm. Similar treatment was done by Friedman in the study of spin-Peierls model.⁵ With these prerequisites, the finite system DMRG algorithm can be implemented in the following way.

As the standard finite system DMRG algorithm which is used in Heisenberg model,¹ the first step of the algorithm is “warmup”. We must generate a series of phonon blocks for the subsequent sweeping processes of the finite system DMRG algorithm. For simplicity, we assume the number of phonon modes is odd and generate the blocks $1 \sim (N-1)/2$ and $(N+3)/2 \sim N$ separately, where different numbers represent different phonon modes. With this simplification, all the phonon blocks $1 \sim 2, 1 \sim 3, \dots, 1 \sim (N-1)/2, (N+3)/2 \sim N, (N+5)/2 \sim N, \dots, N-1 \sim N$ except for the blocks 1 and N which keep N_b bare phonon states are limited to a 2×2 matrix because only the two-state system have been traced out;²¹ see Fig. 1(a). During the course of warmup, each phonon mode with N_b bare phonon states is added to the preceding block. After a truncation with density matrix approach, one new block is generated. We shall show that $N_b = 10$ is sufficient for the implementation of our algorithm in most cases. Note that, every block generated within the warmup processes must be stored in memory for later use.

Secondly, the finite system DMRG algorithm is implemented as in Fig. 1(b). The finite system DMRG algorithm is more or less the same as the standard algorithm.¹ The main difference between the two algorithms is that we add one site within each DMRG step instead of two sites. It is because there are no interactions between the phonon blocks, the implementation of our algorithm is identical to the standard algorithm, and no further correction is needed.²² For convenience, the two-state system can be placed on leftmost side or rightmost side on the chain, as to calculate the reduced density matrix and apply the traditional wave function transformations technique to the finite system algorithm.²³ Within each DMRG step, a phonon mode with N_b bare states is added. This new site is used to generate a new phonon

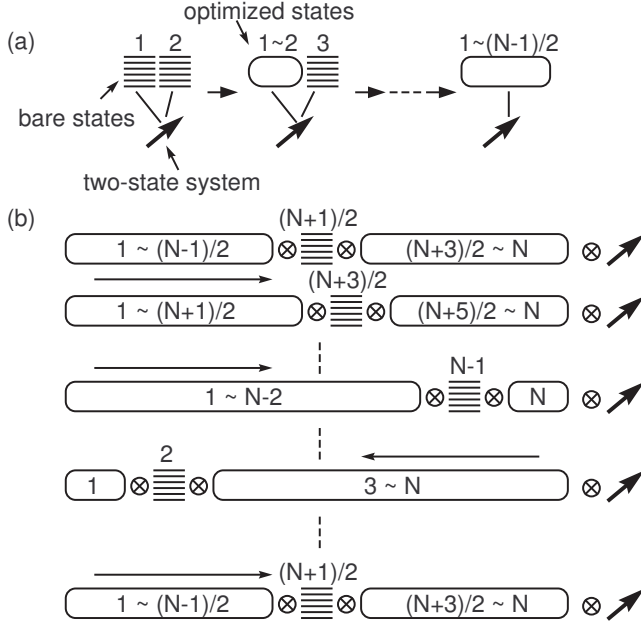


FIG. 1: (a) the warmup procedure of the finite system DMRG algorithm, where the numbers represent the phonon modes. This figure shows the warmup procedure of the left part phonon modes $1 \sim (N-1)/2$; see Fig. 1(b). The right part phonon modes can be obtained by similar fashion. (b) Systematic illustration of the finite system DMRG algorithm. This figure shows one sweep in the algorithm.

block or optimize the old phonon block with M optimized states. Finally, the energies of the target states will converge after one or two sweeps are preformed.

In summary, the algorithm can be proceeded as follows:

1. warmup, generating a series of phonon blocks for subsequent sweeping processes;
2. starting at the center phonon mode $(N+1)/2$, adding one phonon mode with N_b bare states to the chain;
3. performing the sweeping process to the whole chain;
4. if the energies of the target states are not converged after a sweeping, then return to step (2).

III. DISCUSSION AND THE LIMITATION OF THE ALGORITHM

One important issue of the algorithm is that how to choose the parameters N, N_b, M , and the number of sweeps N_s . Unlike the spin $1/2$ Heisenberg chain, there are no interactions between the phonon blocks, the number of states kept per block is not quite large. Therefore, it may be possible to treat a thousand phonon modes while the number of states kept per block is never needed

more than $M = 20 \sim 30$. In general, there are only 7–8 largest eigenvalues in the reduced density matrix of the phonon block have significant values. The dependence

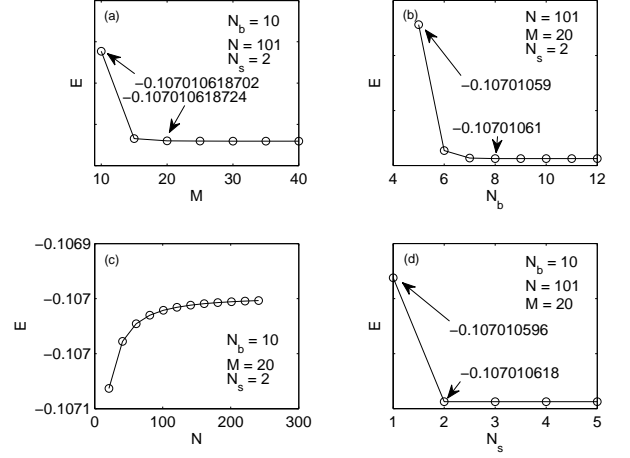


FIG. 2: Dependence of the ground state energy on the parameters N, N_b, M , and N_s for $\epsilon = 0, s = 0.6, \alpha = 0.1$, and $\Delta = 0.1$. (a) dependence on M for fixed N, N_b , and N_s ; (b) dependence on N_b for fixed N, M , and N_s ; (c) dependence on the number of phonon modes N for fixed N_b, M , and N_s ; (d) dependence on N_s , the number of sweeps versus the ground state energy, for fixed N_b, N , and M .

of the ground state energy on the parameters N, N_b, M , and N_s for $s = 0.6, \alpha = 0.1$, and $\Delta = 0.1$ is shown in Fig. 2 (targeting the ground state only, but the following conclusions are also true for targeting both the ground state and the first excited state). It is worth noting that even though $M = 10, N_b = 6$, and $N_s = 1$ can give rather the same results. However, the number of phonon modes N will highly affect the results. This is also the main limitation of our DMRG strategy.

As indicated in Refs. 6, 15, and 24, the very small energy phonon modes are important for revealing the critical phenomena, e.g., the delocalized-localized transition of the two-state system. However, the strategy of our algorithm needs linear discretization of the spectrum which can not resolve very small energy scale. If one tries to apply a logarithmic discretization which is used in NRG to the DMRG algorithm, the energy levels of the Hamiltonian emerge a staircase-like aspect when one deals with the very small energy phonon modes; see Fig. 3. The DMRG scheme fails in this situation because the target states cannot be determined. This difficulty stems from the truncation strategy of the DMRG, say, it iteratively calculates the lowest eigenstates for finding the most probable states of the decimated system. However, in practice, it is harsh for the iterative diagonalization routines being used by DMRG, such as Lanczos and Davidson, to converge when the staircase-like energy levels occur. In fact, the staircase-like energy levels also appear in NRG calculations. Nevertheless, the truncation

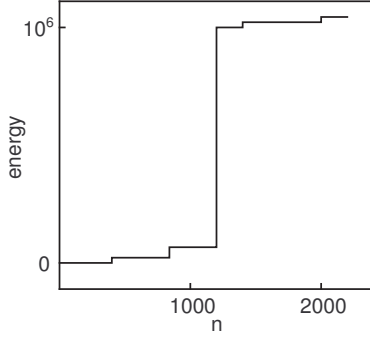


FIG. 3: This figure is a schematic scaled energy spectrum of the DMRG or NRG calculation when one deals with the very small energy phonon modes. Here n is the number of energy levels. The vertical coordinate (energy) is scaled by N and Λ^N in DMRG and NRG, respectively.

scheme of NRG, which retains the lowest-lying states directly, is simply to implement in this situation. In other words, the performance of the standard diagonalization routine used by NRG will not be affected by the “shape” of the spectrum while DMRG needs iterative diagonalization routine which converges arduously.

DMRG cannot resolve very small energy scales, this limitation is serious. It implies that the critical coupling α_c cannot be determined due to the energy levels cannot reach a fixed point without very small energy phonons¹⁵ and the spin-spin correlation function cannot be calculated in very small energy scales. Furthermore, the effective tunneling splitting $\Delta_r = \langle \sigma_x \rangle$ also is not adequate to identify the critical coupling α_c because it fails to characterize the tunneling in equilibrium in the sub-Ohmic case.²⁵ Our DMRG calculations have the same conclusion, namely, $\Delta_r \neq 0$ when $\alpha > \alpha_c$ in the sub-Ohmic case and $\Delta_r \rightarrow 0$ when $\alpha \rightarrow \alpha_c$ (note that α_c is a function of s and Δ) in the Ohmic case (not presented). Moreover, the entanglement entropy method proposed by Ref. 26 recently, which is used to determine the critical couplings and performs very well in NRG, is not working as expected in DMRG when the very small energy information is lacking.

IV. EXTRACTING THE CRITICAL POINTS BY EXTRAPOLATION

Now, we seek to show that the critical couplings α_c can be determined by extrapolating the pseudo-critical couplings α'_c which are extracted in a “DMRG flow” to thermodynamic limit.²⁷ Similar to the energies in logarithmic discretization of NRG which are falling off as Λ^{-N} ,¹⁵ the energies are falling off as N^{-1} in linear discretization. Therefore, one can target the ground state and the first excited state and scale the energy gap $\Delta E = E_{\text{excited}} - E_{\text{ground}}$ as $N\Delta E$ and plot the flow diagram $N\Delta E$ versus N . As one can see in Fig. 4, the flows

of $N\Delta E$ are qualitatively different within two regime $\alpha < \alpha_c$ and $\alpha > \alpha_c$. Therefore, we assume that there

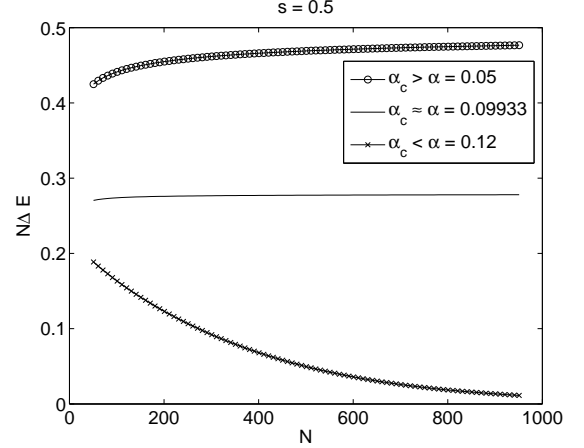


FIG. 4: Dependence of the scaled energy different between ground state and excited state $N\Delta E$ on the number of phonon modes N for $\alpha < \alpha_c$, $\alpha \approx \alpha_c$, and $\alpha > \alpha_c$. Parameters are $\epsilon = 0$, $s = 0.5$, $N_b = 10$, $M = 20$, and $N_s = 2$.

exist a function $\alpha'_c(N)$ which separates the two regimes, where N is relatively small in comparison with thermodynamic limit. In practice, $\alpha'_c(N)$ can be easily determined by a bisection process of two couplings $\alpha < \alpha'_c(N)$ and $\alpha > \alpha'_c(N)$ with the slope of a line segment consist of the scaled energies of two points $[N-1, N+1]$. We conceive that the pseudo-critical coupling $\alpha'_c(N)$ will converge to the critical coupling α_c when $N \rightarrow \infty$ since the fixed points are reached.

Accordingly, the extrapolation of the $\alpha'_c(N)$ versus $1/N$ curve determines the critical coupling α_c at the limit of $1/N \rightarrow 0$. Figure 5 shows the best-fit of the pseudo-

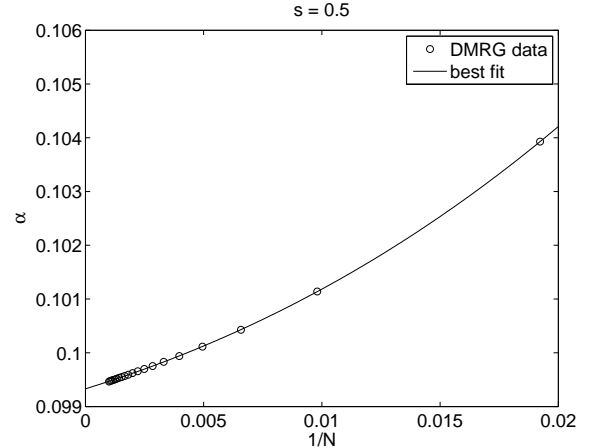


FIG. 5: Dependence of the pseudo-critical couplings $\alpha'_c(N)$ (circle) and the best-fit values (line) on the inverse number of phonon modes $1/N$. Parameters are $\epsilon = 0$, $s = 0.5$, $N_b = 10$, $M = 20$, and $N_s = 2$.

critical couplings $\alpha'_c(N)$ with $s = 0.5$. At $1/N = 0$,

it turns out that $\alpha_c \approx 0.09933$. In fact, the best-fit curves $\alpha'_c(1/N)$ are somewhat different for sub-Ohmic and Ohmic dissipation. It is related to the fact that the transition in the sub-Ohmic case is characterized by a quantum critical fixed point in contrast to the Ohmic case.¹⁵ Since we cannot find a formula to fit all the cases, the extrapolations are done by the simplest polynomial fitting.

Admittedly, it might be doubted that if N is small, α'_c could be inappropriate for extrapolation since it is inconsistent with the α'_c which are obtained with large N . For instance, there are some cases show that the infinite system DMRG is a better choice to tackle this problem.^{28,29,30} However, on the one hand, our strategy of the DMRG in the spin-boson model limits the implementation of the algorithm. In order to “insert” the spin-boson model into the DMRG algorithm, one must cut the spectrum of the bosonic bath to finite number of pieces and therefore the spin-boson model becomes a finite-size chain. Before performing the linear discretization, the number of sites N and the coupling constant λ_i must be determined. Naturally, it brings about the finite system DMRG algorithm to handle this model and a “real” infinite DMRG algorithm is difficult to implement in practice. On the other hand, in our finite system DMRG solution, the number of phonon modes treated is relatively large. We carefully check the calculations and find that when we calculate the α'_c with $1/N \leq 0.005$, the α'_c are always monotonic. Hence, the extrapolations are safe and correct in our treatment. Furthermore, references 28 and 29 also performed an extrapolation of the number of states kept, but the result shown in Fig. 2 and the fact of non-interacting phonon blocks guarantee that this quantity is not significant in our calculation notwithstanding.

Using the extrapolation scheme, the phase boundary for the delocalized-localized transition of the spin-boson model for $\epsilon = 0$ and $\Delta = 0.1$ is shown in Fig. 6, where the result by NRG is also shown for comparison. It can be found that the DMRG data are consistent with the NRG data quite well. It also shows that the NRG data are always larger than the DMRG data. Indeed, however, the results of NRG can be extrapolated to thermodynamics limit, namely, one takes the NRG discretization parameter $\Lambda \rightarrow 1$, and smaller critical couplings can be obtained.¹⁵ In other words, both NRG and DMRG show that the critical couplings before extrapolating to thermodynamics limit are always larger than the true critical couplings. This implies that the error of discretiza-

tion on determining the critical coupling is to lower the true α_c , but not to heighten the α_c as claimed in Ref. 14. In addition, the inset of Fig. 6 also assures that our DMRG calculations for Ohmic case are consistent with the NRG result¹⁵ and the well-known renormalization group result,⁷ i.e., $\alpha_c = 1 + \mathcal{O}(\Delta/\omega_c)$.

V. CONCLUSION

At the end of this paper, we want to compare the ground state energy obtained by DMRG with the variational ground state energy obtained by displaced-oscillator approach. As we mentioned in the Introduction, the variational ground state will fail at a certain point since the variational ground state is not yet stable.^{13,19} The comparison of the ground state energy is shown in Fig. 7. It shows that the DMRG ground state energies are always lower than that of the variational calculations. It is also clear that the DMRG ground state energy approaches to variational ground state energy for small α and displaced-oscillator ground state energy for large α , and no discontinuous effective tunneling splitting and ground state energy are observed by the DMRG calculations.

In conclusion, we have proposed a finite system DMRG algorithm to deal with the spin-boson model. This algorithm is much more powerful than the preceding study of this topic because it can treat more than a thousand phonon modes.⁶ In fact, we have tried to calculate 10^4 and 10^5 phonon modes. Unfortunately, our 32-bit system is unable to tackle phonon modes on the 10^5 magnitude due to out of memory. This difficulty, of course, can be resolved in 64-bit system or storing the data in hard disk. Moreover, we obtain the critical couplings α_c by extrapolating the pseudo-critical couplings to thermodynamic limit. The phase diagram is compared with NRG and shows good agreement in both sub-Ohmic and Ohmic cases.

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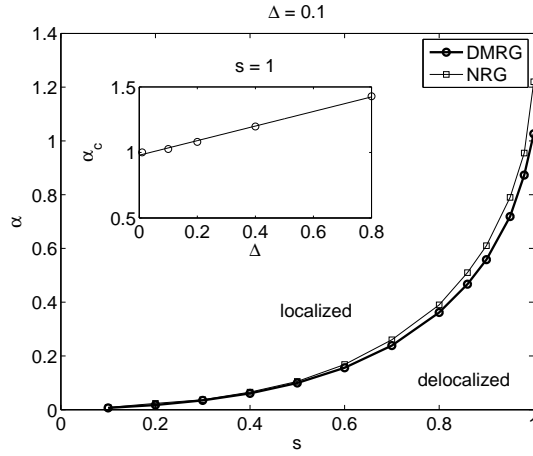


FIG. 6: The delocalized-localized transition boundary of the spin-boson model. The DMRG data are compared with the NRG data (Ref. 15, PRL). Inset: dependence of the α_c on the parameter Δ for Ohmic case and the related linear fit $\alpha_c(\Delta) = 0.56\Delta + 0.98$. Parameters are $\epsilon = 0$, $N_b = 10$, $M = 20$, and $N_s = 2$.

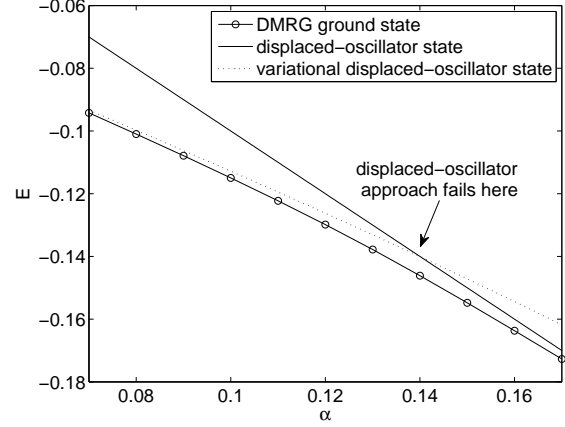


FIG. 7: This figure shows the ground state energy comparison of the DMRG and variational approach for $\epsilon = 0$, $s = 0.5$, and $\Delta = 0.1$. DMRG parameters are $N = 201$, $N_b = 30$, $M = 20$, and $N_s = 2$.

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